



wwPDB EM Validation Summary Report ⓘ

Nov 24, 2022 – 06:26 AM EST

PDB ID : 7T4R
EMDB ID : EMD-25686
Title : CryoEM structure of the HCMV Pentamer gH/gL/UL128/UL130/UL131A in complex with THBD and neutralizing fabs MSL-109 and 13H11
Authors : Kschonsak, M.; Johnson, M.C.; Schelling, R.; Green, E.M.; Rouge, L.; Ho, H.; Patel, N.; Kilic, C.; Kraft, E.; Arthur, C.P.; Rohou, A.L.; Comps-Agrar, L.; Martinez-Martin, N.; Perez, L.; Payandeh, J.; Ciferri, C.
Deposited on : 2021-12-10
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

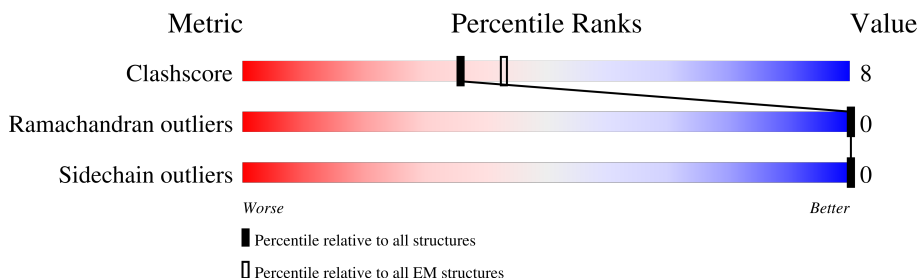
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






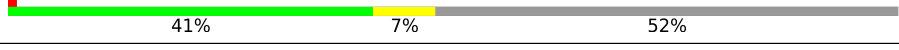

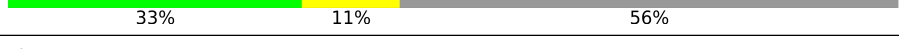

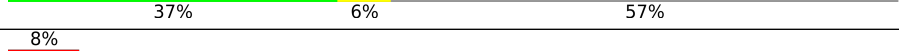
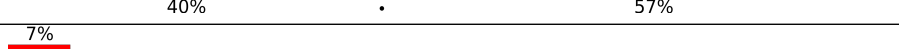
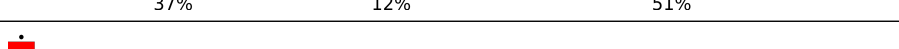
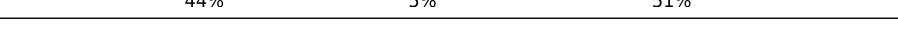
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	
2	B	767	
2	K	767	
3	C	278	
3	L	278	
4	D	171	
4	M	171	
5	E	254	

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Mol	Chain	Length	Quality of chain
5	N	254	 48% 16% 36%
6	F	129	 70% 15% 16%
6	O	129	 67% 15% 19%
7	G	250	 41% 7% 52%
7	P	250	 42% 6% 52%
8	H	237	 33% 11% 56%
8	Q	237	 39% 5% 56%
9	I	257	 16% 37% 6% 57%
9	R	257	 8% 40% 57%
10	J	257	 7% 37% 12% 51%
10	S	257	 44% 5% 51%

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 28717 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Thrombomodulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	144	1083	680	193	200	10	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	517	GLY	-	expression tag	UNP P07204
A	518	ASN	-	expression tag	UNP P07204
A	519	SER	-	expression tag	UNP P07204
A	520	ASP	-	expression tag	UNP P07204
A	521	TYR	-	expression tag	UNP P07204
A	522	LYS	-	expression tag	UNP P07204
A	523	ASP	-	expression tag	UNP P07204
A	524	ASP	-	expression tag	UNP P07204
A	525	ASP	-	expression tag	UNP P07204
A	526	ASP	-	expression tag	UNP P07204
A	527	LYS	-	expression tag	UNP P07204

- Molecule 2 is a protein called Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	630	5075	3257	857	936	25	0	0
2	K	633	5097	3267	861	944	25	0	0

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	716	GLY	-	expression tag	UNP F5H9T3
B	717	THR	-	expression tag	UNP F5H9T3
B	718	LYS	-	expression tag	UNP F5H9T3
B	719	LEU	-	expression tag	UNP F5H9T3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	720	GLY	-	expression tag	UNP F5H9T3
B	721	PRO	-	expression tag	UNP F5H9T3
B	722	GLU	-	expression tag	UNP F5H9T3
B	723	GLN	-	expression tag	UNP F5H9T3
B	724	LYS	-	expression tag	UNP F5H9T3
B	725	LEU	-	expression tag	UNP F5H9T3
B	726	ILE	-	expression tag	UNP F5H9T3
B	727	SER	-	expression tag	UNP F5H9T3
B	728	GLU	-	expression tag	UNP F5H9T3
B	729	GLU	-	expression tag	UNP F5H9T3
B	730	ASP	-	expression tag	UNP F5H9T3
B	731	LEU	-	expression tag	UNP F5H9T3
B	732	ASN	-	expression tag	UNP F5H9T3
B	733	SER	-	expression tag	UNP F5H9T3
B	734	ALA	-	expression tag	UNP F5H9T3
B	735	VAL	-	expression tag	UNP F5H9T3
B	736	ASP	-	expression tag	UNP F5H9T3
B	737	GLY	-	expression tag	UNP F5H9T3
B	738	SER	-	expression tag	UNP F5H9T3
B	739	GLY	-	expression tag	UNP F5H9T3
B	740	LEU	-	expression tag	UNP F5H9T3
B	741	ASN	-	expression tag	UNP F5H9T3
B	742	ASP	-	expression tag	UNP F5H9T3
B	743	ILE	-	expression tag	UNP F5H9T3
B	744	PHE	-	expression tag	UNP F5H9T3
B	745	GLU	-	expression tag	UNP F5H9T3
B	746	ALA	-	expression tag	UNP F5H9T3
B	747	GLN	-	expression tag	UNP F5H9T3
B	748	LYS	-	expression tag	UNP F5H9T3
B	749	ILE	-	expression tag	UNP F5H9T3
B	750	GLU	-	expression tag	UNP F5H9T3
B	751	TRP	-	expression tag	UNP F5H9T3
B	752	HIS	-	expression tag	UNP F5H9T3
B	753	GLU	-	expression tag	UNP F5H9T3
B	754	ASN	-	expression tag	UNP F5H9T3
B	755	LEU	-	expression tag	UNP F5H9T3
B	756	TYR	-	expression tag	UNP F5H9T3
B	757	PHE	-	expression tag	UNP F5H9T3
B	758	GLN	-	expression tag	UNP F5H9T3
B	759	GLY	-	expression tag	UNP F5H9T3
B	760	HIS	-	expression tag	UNP F5H9T3
B	761	HIS	-	expression tag	UNP F5H9T3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	762	HIS	-	expression tag	UNP F5H9T3
B	763	HIS	-	expression tag	UNP F5H9T3
B	764	HIS	-	expression tag	UNP F5H9T3
B	765	HIS	-	expression tag	UNP F5H9T3
B	766	HIS	-	expression tag	UNP F5H9T3
B	767	HIS	-	expression tag	UNP F5H9T3
K	716	GLY	-	expression tag	UNP F5H9T3
K	717	THR	-	expression tag	UNP F5H9T3
K	718	LYS	-	expression tag	UNP F5H9T3
K	719	LEU	-	expression tag	UNP F5H9T3
K	720	GLY	-	expression tag	UNP F5H9T3
K	721	PRO	-	expression tag	UNP F5H9T3
K	722	GLU	-	expression tag	UNP F5H9T3
K	723	GLN	-	expression tag	UNP F5H9T3
K	724	LYS	-	expression tag	UNP F5H9T3
K	725	LEU	-	expression tag	UNP F5H9T3
K	726	ILE	-	expression tag	UNP F5H9T3
K	727	SER	-	expression tag	UNP F5H9T3
K	728	GLU	-	expression tag	UNP F5H9T3
K	729	GLU	-	expression tag	UNP F5H9T3
K	730	ASP	-	expression tag	UNP F5H9T3
K	731	LEU	-	expression tag	UNP F5H9T3
K	732	ASN	-	expression tag	UNP F5H9T3
K	733	SER	-	expression tag	UNP F5H9T3
K	734	ALA	-	expression tag	UNP F5H9T3
K	735	VAL	-	expression tag	UNP F5H9T3
K	736	ASP	-	expression tag	UNP F5H9T3
K	737	GLY	-	expression tag	UNP F5H9T3
K	738	SER	-	expression tag	UNP F5H9T3
K	739	GLY	-	expression tag	UNP F5H9T3
K	740	LEU	-	expression tag	UNP F5H9T3
K	741	ASN	-	expression tag	UNP F5H9T3
K	742	ASP	-	expression tag	UNP F5H9T3
K	743	ILE	-	expression tag	UNP F5H9T3
K	744	PHE	-	expression tag	UNP F5H9T3
K	745	GLU	-	expression tag	UNP F5H9T3
K	746	ALA	-	expression tag	UNP F5H9T3
K	747	GLN	-	expression tag	UNP F5H9T3
K	748	LYS	-	expression tag	UNP F5H9T3
K	749	ILE	-	expression tag	UNP F5H9T3
K	750	GLU	-	expression tag	UNP F5H9T3
K	751	TRP	-	expression tag	UNP F5H9T3

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Chain	Residue	Modelled	Actual	Comment	Reference
K	752	HIS	-	expression tag	UNP F5H9T3
K	753	GLU	-	expression tag	UNP F5H9T3
K	754	ASN	-	expression tag	UNP F5H9T3
K	755	LEU	-	expression tag	UNP F5H9T3
K	756	TYR	-	expression tag	UNP F5H9T3
K	757	PHE	-	expression tag	UNP F5H9T3
K	758	GLN	-	expression tag	UNP F5H9T3
K	759	GLY	-	expression tag	UNP F5H9T3
K	760	HIS	-	expression tag	UNP F5H9T3
K	761	HIS	-	expression tag	UNP F5H9T3
K	762	HIS	-	expression tag	UNP F5H9T3
K	763	HIS	-	expression tag	UNP F5H9T3
K	764	HIS	-	expression tag	UNP F5H9T3
K	765	HIS	-	expression tag	UNP F5H9T3
K	766	HIS	-	expression tag	UNP F5H9T3
K	767	HIS	-	expression tag	UNP F5H9T3

- Molecule 3 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	233	Total	C	N	O	S	0	0
			1843	1173	322	340	8		
3	L	230	Total	C	N	O	S	0	0
			1818	1157	318	335	8		

- Molecule 4 is a protein called Envelope protein UL128.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	129	Total	C	N	O	S	0	0
			1038	651	190	188	9		
4	M	132	Total	C	N	O	S	0	0
			1067	673	193	190	11		

- Molecule 5 is a protein called Envelope glycoprotein UL130.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	163	Total	C	N	O	S	0	0
			1327	847	233	239	8		
5	N	163	Total	C	N	O	S	0	0
			1328	846	233	241	8		

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	215	GLY	-	expression tag	UNP Q38M07
E	216	SER	-	expression tag	UNP Q38M07
E	217	GLU	-	expression tag	UNP Q38M07
E	218	ASN	-	expression tag	UNP Q38M07
E	219	LEU	-	expression tag	UNP Q38M07
E	220	TYR	-	expression tag	UNP Q38M07
E	221	PHE	-	expression tag	UNP Q38M07
E	222	GLN	-	expression tag	UNP Q38M07
E	223	GLY	-	expression tag	UNP Q38M07
E	224	SER	-	expression tag	UNP Q38M07
E	225	ALA	-	expression tag	UNP Q38M07
E	226	TRP	-	expression tag	UNP Q38M07
E	227	SER	-	expression tag	UNP Q38M07
E	228	HIS	-	expression tag	UNP Q38M07
E	229	PRO	-	expression tag	UNP Q38M07
E	230	GLN	-	expression tag	UNP Q38M07
E	231	PHE	-	expression tag	UNP Q38M07
E	232	GLU	-	expression tag	UNP Q38M07
E	233	LYS	-	expression tag	UNP Q38M07
E	234	GLY	-	expression tag	UNP Q38M07
E	235	GLY	-	expression tag	UNP Q38M07
E	236	GLY	-	expression tag	UNP Q38M07
E	237	SER	-	expression tag	UNP Q38M07
E	238	GLY	-	expression tag	UNP Q38M07
E	239	GLY	-	expression tag	UNP Q38M07
E	240	GLY	-	expression tag	UNP Q38M07
E	241	SER	-	expression tag	UNP Q38M07
E	242	GLY	-	expression tag	UNP Q38M07
E	243	GLY	-	expression tag	UNP Q38M07
E	244	GLY	-	expression tag	UNP Q38M07
E	245	SER	-	expression tag	UNP Q38M07
E	246	ALA	-	expression tag	UNP Q38M07
E	247	TRP	-	expression tag	UNP Q38M07
E	248	SER	-	expression tag	UNP Q38M07
E	249	HIS	-	expression tag	UNP Q38M07
E	250	PRO	-	expression tag	UNP Q38M07
E	251	GLN	-	expression tag	UNP Q38M07
E	252	PHE	-	expression tag	UNP Q38M07
E	253	GLU	-	expression tag	UNP Q38M07
E	254	LYS	-	expression tag	UNP Q38M07
N	215	GLY	-	expression tag	UNP Q38M07
N	216	SER	-	expression tag	UNP Q38M07
N	217	GLU	-	expression tag	UNP Q38M07

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Chain	Residue	Modelled	Actual	Comment	Reference
N	218	ASN	-	expression tag	UNP Q38M07
N	219	LEU	-	expression tag	UNP Q38M07
N	220	TYR	-	expression tag	UNP Q38M07
N	221	PHE	-	expression tag	UNP Q38M07
N	222	GLN	-	expression tag	UNP Q38M07
N	223	GLY	-	expression tag	UNP Q38M07
N	224	SER	-	expression tag	UNP Q38M07
N	225	ALA	-	expression tag	UNP Q38M07
N	226	TRP	-	expression tag	UNP Q38M07
N	227	SER	-	expression tag	UNP Q38M07
N	228	HIS	-	expression tag	UNP Q38M07
N	229	PRO	-	expression tag	UNP Q38M07
N	230	GLN	-	expression tag	UNP Q38M07
N	231	PHE	-	expression tag	UNP Q38M07
N	232	GLU	-	expression tag	UNP Q38M07
N	233	LYS	-	expression tag	UNP Q38M07
N	234	GLY	-	expression tag	UNP Q38M07
N	235	GLY	-	expression tag	UNP Q38M07
N	236	GLY	-	expression tag	UNP Q38M07
N	237	SER	-	expression tag	UNP Q38M07
N	238	GLY	-	expression tag	UNP Q38M07
N	239	GLY	-	expression tag	UNP Q38M07
N	240	GLY	-	expression tag	UNP Q38M07
N	241	SER	-	expression tag	UNP Q38M07
N	242	GLY	-	expression tag	UNP Q38M07
N	243	GLY	-	expression tag	UNP Q38M07
N	244	GLY	-	expression tag	UNP Q38M07
N	245	SER	-	expression tag	UNP Q38M07
N	246	ALA	-	expression tag	UNP Q38M07
N	247	TRP	-	expression tag	UNP Q38M07
N	248	SER	-	expression tag	UNP Q38M07
N	249	HIS	-	expression tag	UNP Q38M07
N	250	PRO	-	expression tag	UNP Q38M07
N	251	GLN	-	expression tag	UNP Q38M07
N	252	PHE	-	expression tag	UNP Q38M07
N	253	GLU	-	expression tag	UNP Q38M07
N	254	LYS	-	expression tag	UNP Q38M07

- Molecule 6 is a protein called Envelope protein UL131A.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
6	F	109	900	562	169	167	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	105	Total	C	N	O	S	0	0
			869	545	161	162	1		

- Molecule 7 is a protein called Fab 13H11 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	120	Total	C	N	O	S	0	0
			918	578	159	176	5		
7	P	120	Total	C	N	O	S	0	0
			918	578	159	176	5		

- Molecule 8 is a protein called Fab 13H11 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	104	Total	C	N	O	S	0	0
			782	496	130	153	3		
8	Q	104	Total	C	N	O	S	0	0
			782	496	130	153	3		

- Molecule 9 is a protein called Fab MSL-109 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			850	534	143	169	4		
9	R	111	Total	C	N	O	S	0	0
			850	534	143	169	4		

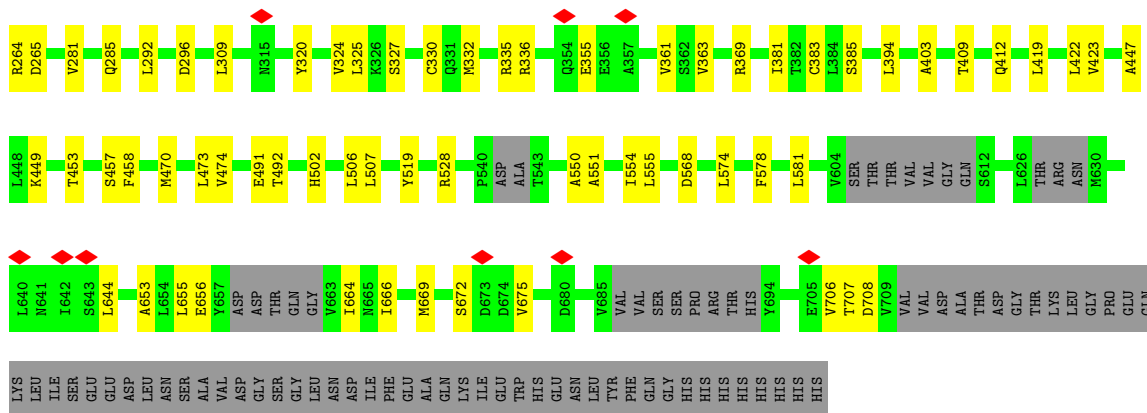
- Molecule 10 is a protein called Fab MSL-109 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	127	Total	C	N	O	S	0	0
			988	627	163	195	3		
10	S	127	Total	C	N	O	S	0	0
			988	627	163	195	3		

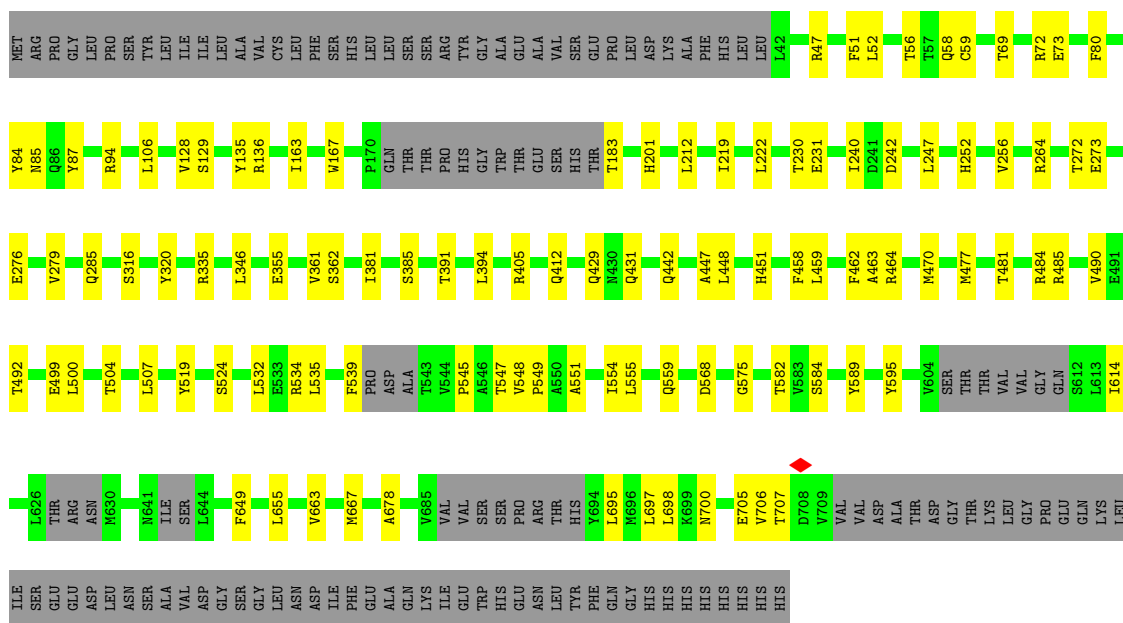
- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



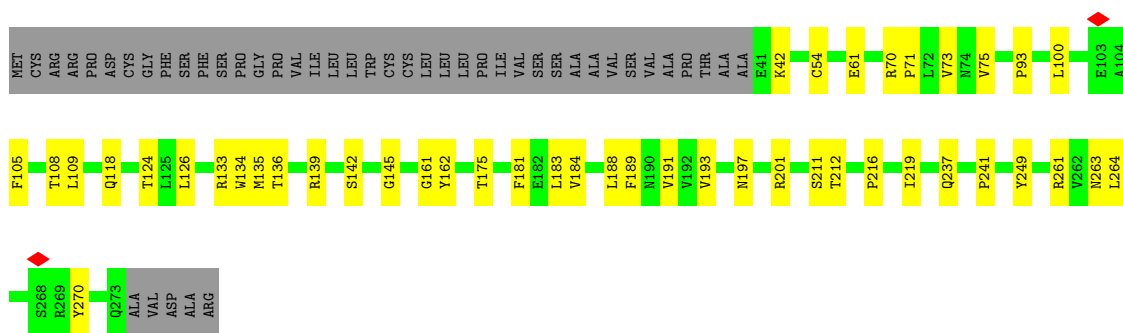
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	B	1	70	40	5	25	0
11	B	1	70	40	5	25	0
11	B	1	70	40	5	25	0
11	B	1	70	40	5	25	0
11	B	1	70	40	5	25	0
11	C	1	14	8	1	5	0
11	E	1	14	8	1	5	0
11	K	1	70	40	5	25	0
11	K	1	70	40	5	25	0
11	K	1	70	40	5	25	0
11	K	1	70	40	5	25	0
11	K	1	70	40	5	25	0
11	N	1	14	8	1	5	0
11	O	1	14	8	1	5	0



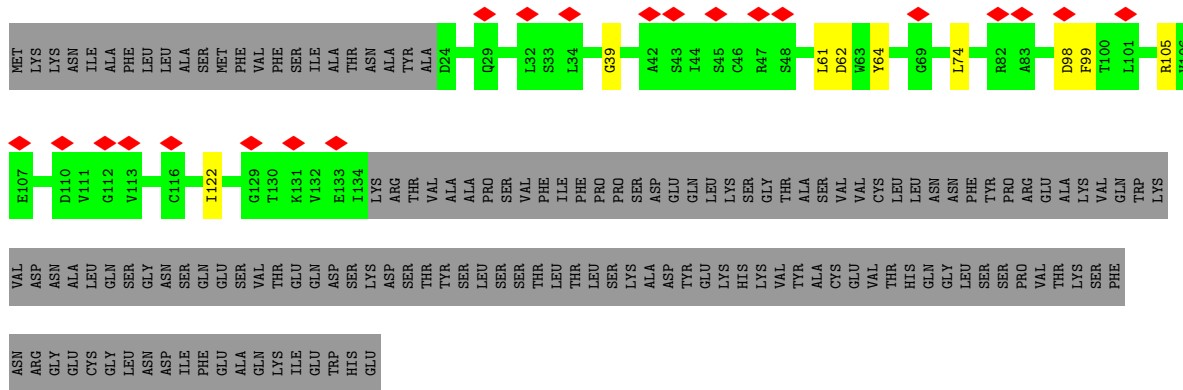
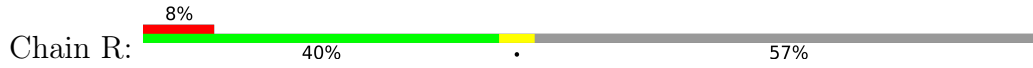
• Molecule 2: Envelope glycoprotein H



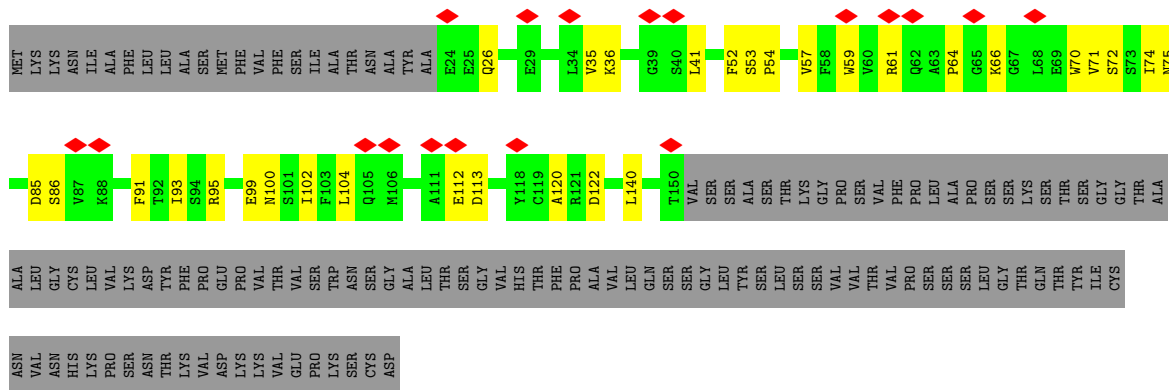
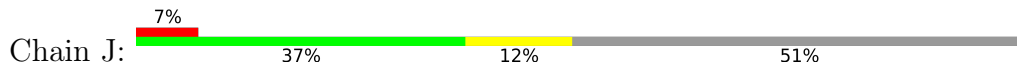
• Molecule 3: Envelope glycoprotein L



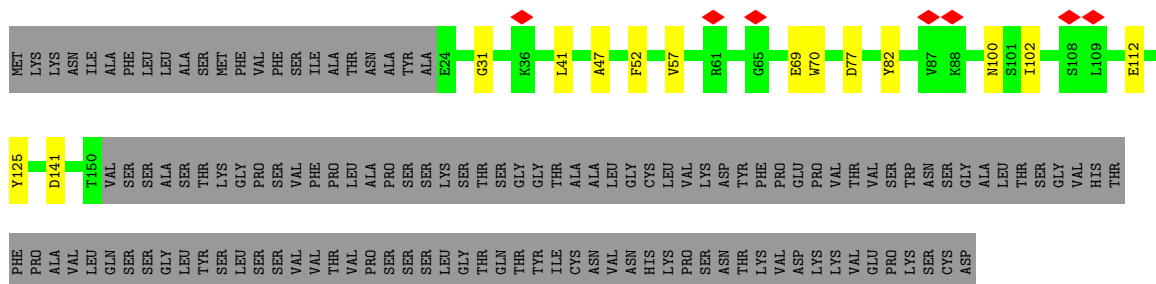
• Molecule 9: Fab MSL-109 light chain



• Molecule 10: Fab MSL-109 heavy chain



• Molecule 10: Fab MSL-109 heavy chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	504492	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.585	Depositor
Minimum map value	-0.474	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	429.04, 429.04, 429.04	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0726, 1.0726, 1.0726	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/1111	0.57	0/1513
2	B	0.28	0/5190	0.52	0/7061
2	K	0.30	0/5212	0.53	0/7091
3	C	0.28	0/1888	0.56	0/2577
3	L	0.30	0/1863	0.56	0/2543
4	D	0.28	0/1059	0.56	0/1432
4	M	0.30	0/1088	0.56	0/1468
5	E	0.35	0/1363	0.59	0/1851
5	N	0.31	0/1364	0.56	0/1852
6	F	0.28	0/920	0.55	0/1245
6	O	0.26	0/889	0.54	0/1204
7	G	0.27	0/938	0.53	0/1272
7	P	0.28	0/938	0.53	0/1272
8	H	0.30	0/800	0.53	0/1089
8	Q	0.28	0/800	0.49	0/1089
9	I	0.26	0/868	0.52	0/1180
9	R	0.26	0/868	0.51	0/1180
10	J	0.28	0/1013	0.53	0/1373
10	S	0.30	0/1013	0.53	0/1373
All	All	0.29	0/29185	0.54	0/39665

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1083	0	1034	28	0
2	B	5075	0	5042	80	0
2	K	5097	0	5051	98	0
3	C	1843	0	1835	36	0
3	L	1818	0	1809	36	0
4	D	1038	0	1038	22	0
4	M	1067	0	1072	29	0
5	E	1327	0	1305	48	0
5	N	1328	0	1300	34	0
6	F	900	0	867	18	0
6	O	869	0	835	16	0
7	G	918	0	895	10	0
7	P	918	0	895	10	0
8	H	782	0	776	16	0
8	Q	782	0	776	10	0
9	I	850	0	831	12	0
9	R	850	0	831	7	0
10	J	988	0	924	22	0
10	S	988	0	924	14	0
11	B	70	0	65	4	0
11	C	14	0	13	0	0
11	E	14	0	13	0	0
11	K	70	0	65	3	0
11	N	14	0	13	0	0
11	O	14	0	13	0	0
All	All	28717	0	28222	483	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 483 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:81:PRO:HA	5:E:85:ASN:HB2	1.43	1.00
2:K:535:LEU:HD23	2:K:548:VAL:HG13	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:442:GLN:OE1	10:S:125:TYR:CE1	2.24	0.90
7:P:6:GLN:OE1	7:P:96:CYS:SG	2.34	0.85
1:A:92:LEU:HB2	1:A:108:PHE:CE2	2.13	0.83

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	140/527 (27%)	133 (95%)	7 (5%)	0	100	100
2	B	616/767 (80%)	588 (96%)	28 (4%)	0	100	100
2	K	619/767 (81%)	595 (96%)	24 (4%)	0	100	100
3	C	231/278 (83%)	218 (94%)	13 (6%)	0	100	100
3	L	228/278 (82%)	216 (95%)	12 (5%)	0	100	100
4	D	127/171 (74%)	124 (98%)	3 (2%)	0	100	100
4	M	128/171 (75%)	124 (97%)	4 (3%)	0	100	100
5	E	161/254 (63%)	158 (98%)	3 (2%)	0	100	100
5	N	161/254 (63%)	154 (96%)	7 (4%)	0	100	100
6	F	107/129 (83%)	106 (99%)	1 (1%)	0	100	100
6	O	103/129 (80%)	102 (99%)	1 (1%)	0	100	100
7	G	118/250 (47%)	117 (99%)	1 (1%)	0	100	100
7	P	118/250 (47%)	116 (98%)	2 (2%)	0	100	100
8	H	102/237 (43%)	99 (97%)	3 (3%)	0	100	100
8	Q	102/237 (43%)	100 (98%)	2 (2%)	0	100	100
9	I	109/257 (42%)	102 (94%)	7 (6%)	0	100	100
9	R	109/257 (42%)	103 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	125/257 (49%)	120 (96%)	5 (4%)	0	100	100
10	S	125/257 (49%)	120 (96%)	5 (4%)	0	100	100
All	All	3529/5727 (62%)	3395 (96%)	134 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	115/413 (28%)	115 (100%)	0	100	100
2	B	573/692 (83%)	573 (100%)	0	100	100
2	K	575/692 (83%)	575 (100%)	0	100	100
3	C	202/238 (85%)	202 (100%)	0	100	100
3	L	199/238 (84%)	199 (100%)	0	100	100
4	D	115/153 (75%)	115 (100%)	0	100	100
4	M	119/153 (78%)	119 (100%)	0	100	100
5	E	149/223 (67%)	149 (100%)	0	100	100
5	N	149/223 (67%)	149 (100%)	0	100	100
6	F	96/114 (84%)	96 (100%)	0	100	100
6	O	93/114 (82%)	93 (100%)	0	100	100
7	G	100/211 (47%)	100 (100%)	0	100	100
7	P	100/211 (47%)	100 (100%)	0	100	100
8	H	87/204 (43%)	87 (100%)	0	100	100
8	Q	87/204 (43%)	87 (100%)	0	100	100
9	I	97/225 (43%)	97 (100%)	0	100	100
9	R	97/225 (43%)	97 (100%)	0	100	100
10	J	104/216 (48%)	104 (100%)	0	100	100
10	S	104/216 (48%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3161/4965 (64%)	3161 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	K	442	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	NAG	K	801	-	14,14,15	0.18	0	17,19,21	0.44	0
11	NAG	B	803	2	14,14,15	0.17	0	17,19,21	0.43	0
11	NAG	B	801	-	14,14,15	0.23	0	17,19,21	0.93	1 (5%)
11	NAG	B	805	2	14,14,15	0.24	0	17,19,21	0.50	0
11	NAG	B	802	2	14,14,15	0.20	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	K	805	-	14,14,15	0.19	0	17,19,21	0.45	0
11	NAG	K	804	2	14,14,15	0.23	0	17,19,21	0.50	0
11	NAG	N	301	5	14,14,15	0.16	0	17,19,21	0.54	0
11	NAG	E	301	5	14,14,15	0.18	0	17,19,21	0.47	0
11	NAG	K	803	2	14,14,15	0.17	0	17,19,21	0.46	0
11	NAG	K	802	2	14,14,15	0.26	0	17,19,21	0.82	1 (5%)
11	NAG	B	804	2	14,14,15	0.20	0	17,19,21	0.90	1 (5%)
11	NAG	C	301	3	14,14,15	0.22	0	17,19,21	0.41	0
11	NAG	O	201	6	14,14,15	0.24	0	17,19,21	0.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	K	801	-	-	3/6/23/26	0/1/1/1
11	NAG	B	803	2	-	4/6/23/26	0/1/1/1
11	NAG	B	801	-	-	6/6/23/26	0/1/1/1
11	NAG	B	805	2	-	2/6/23/26	0/1/1/1
11	NAG	B	802	2	-	2/6/23/26	0/1/1/1
11	NAG	K	805	-	-	1/6/23/26	0/1/1/1
11	NAG	K	804	2	-	2/6/23/26	0/1/1/1
11	NAG	N	301	5	-	3/6/23/26	0/1/1/1
11	NAG	E	301	5	-	2/6/23/26	0/1/1/1
11	NAG	K	803	2	-	4/6/23/26	0/1/1/1
11	NAG	K	802	2	-	4/6/23/26	0/1/1/1
11	NAG	B	804	2	-	5/6/23/26	0/1/1/1
11	NAG	C	301	3	-	1/6/23/26	0/1/1/1
11	NAG	O	201	6	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	802	NAG	C1-O5-C5	3.13	116.43	112.19
11	B	804	NAG	C2-N2-C7	2.72	126.78	122.90
11	B	801	NAG	C2-N2-C7	2.69	126.73	122.90

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	802	NAG	C1-C2-N2-C7
11	K	805	NAG	C3-C2-N2-C7
11	B	805	NAG	O5-C5-C6-O6
11	E	301	NAG	O5-C5-C6-O6
11	K	804	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	801	NAG	2	0
11	K	804	NAG	1	0
11	K	802	NAG	2	0
11	B	804	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

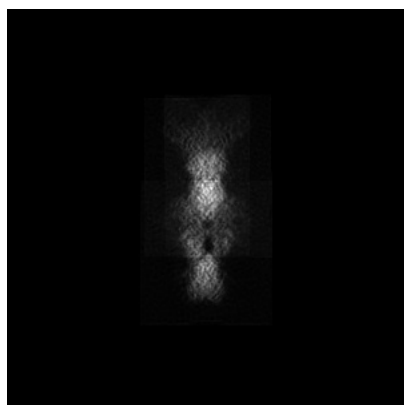
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25686. These allow visual inspection of the internal detail of the map and identification of artifacts.

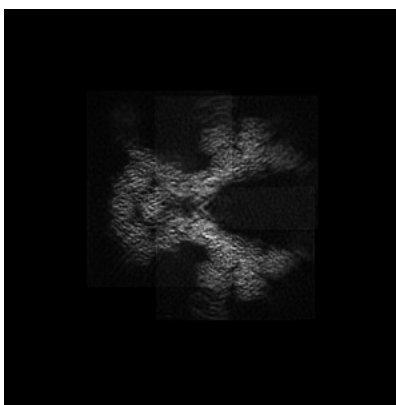
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

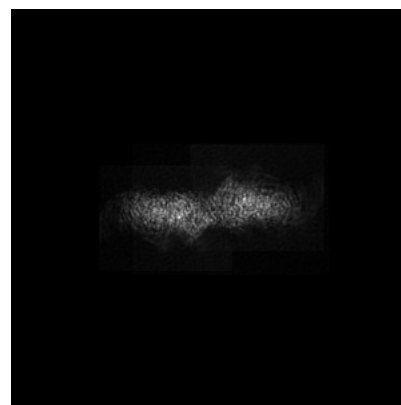
6.1.1 Primary map



X



Y

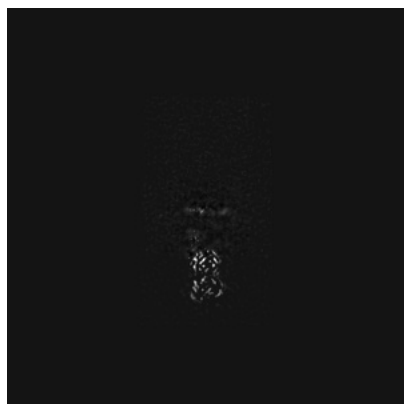


Z

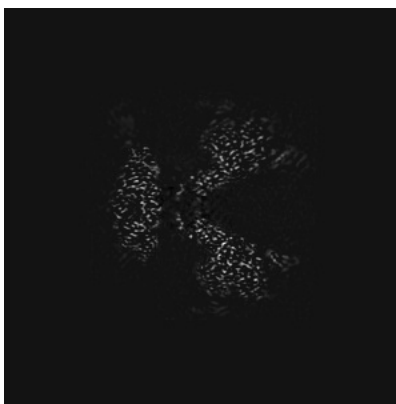
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

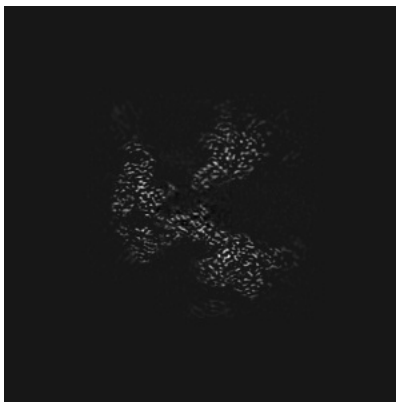
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

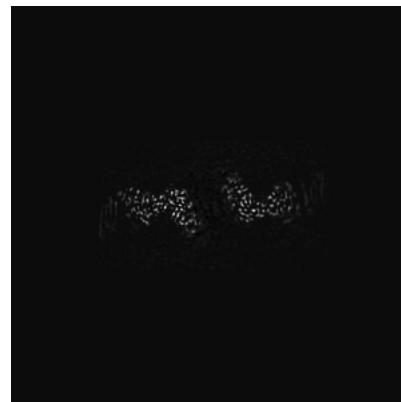
6.3.1 Primary map



X Index: 170



Y Index: 195



Z Index: 211

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

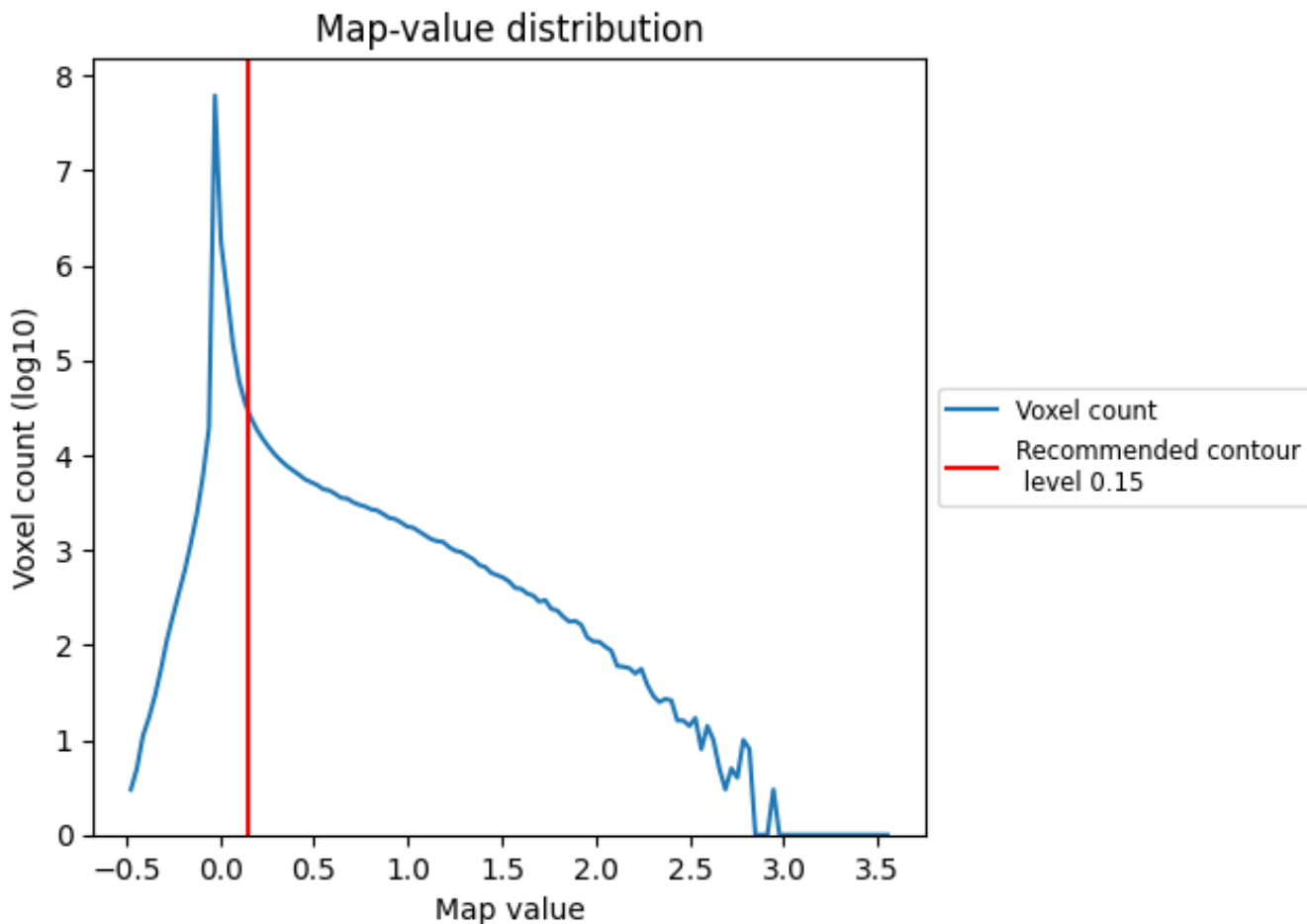
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

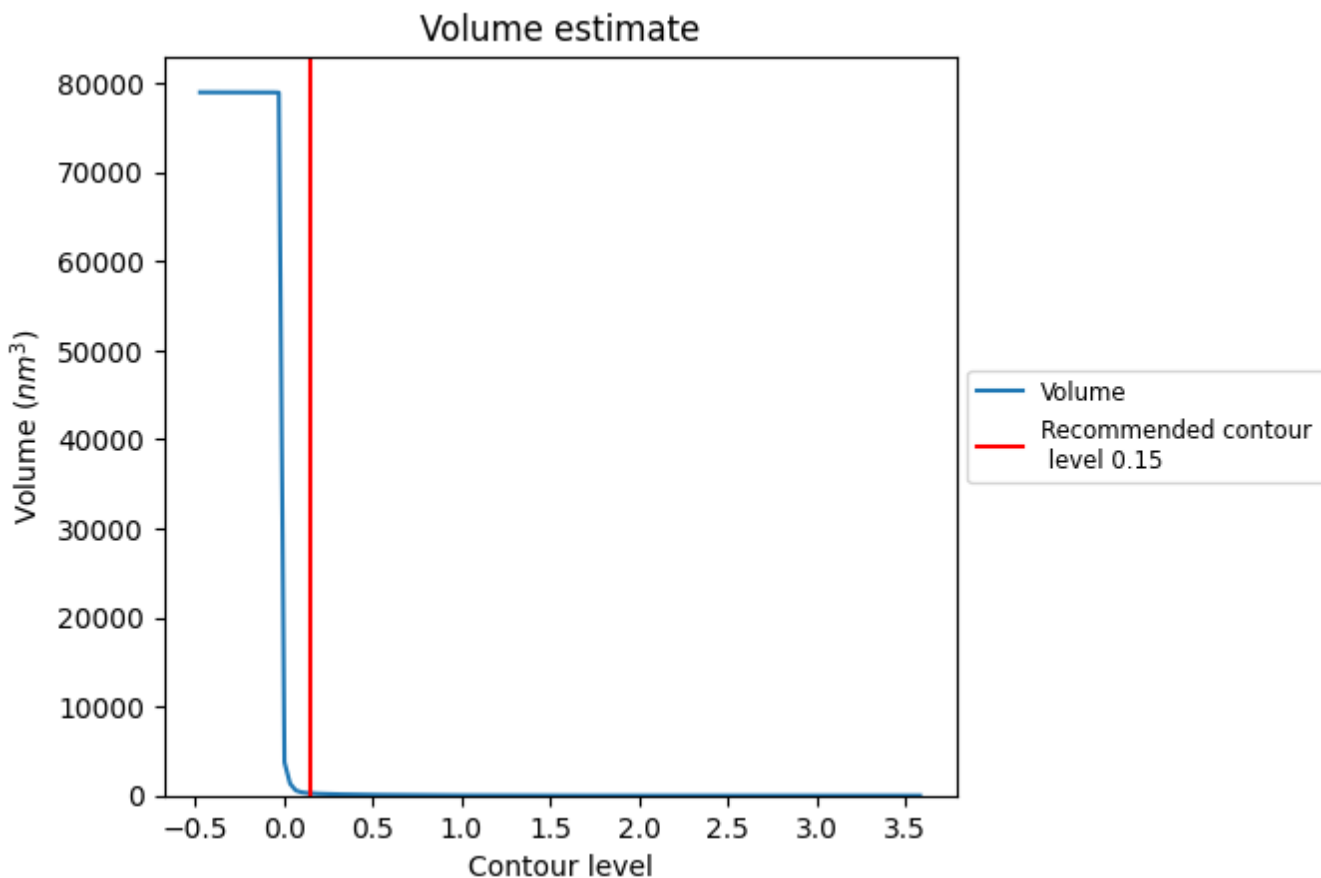
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

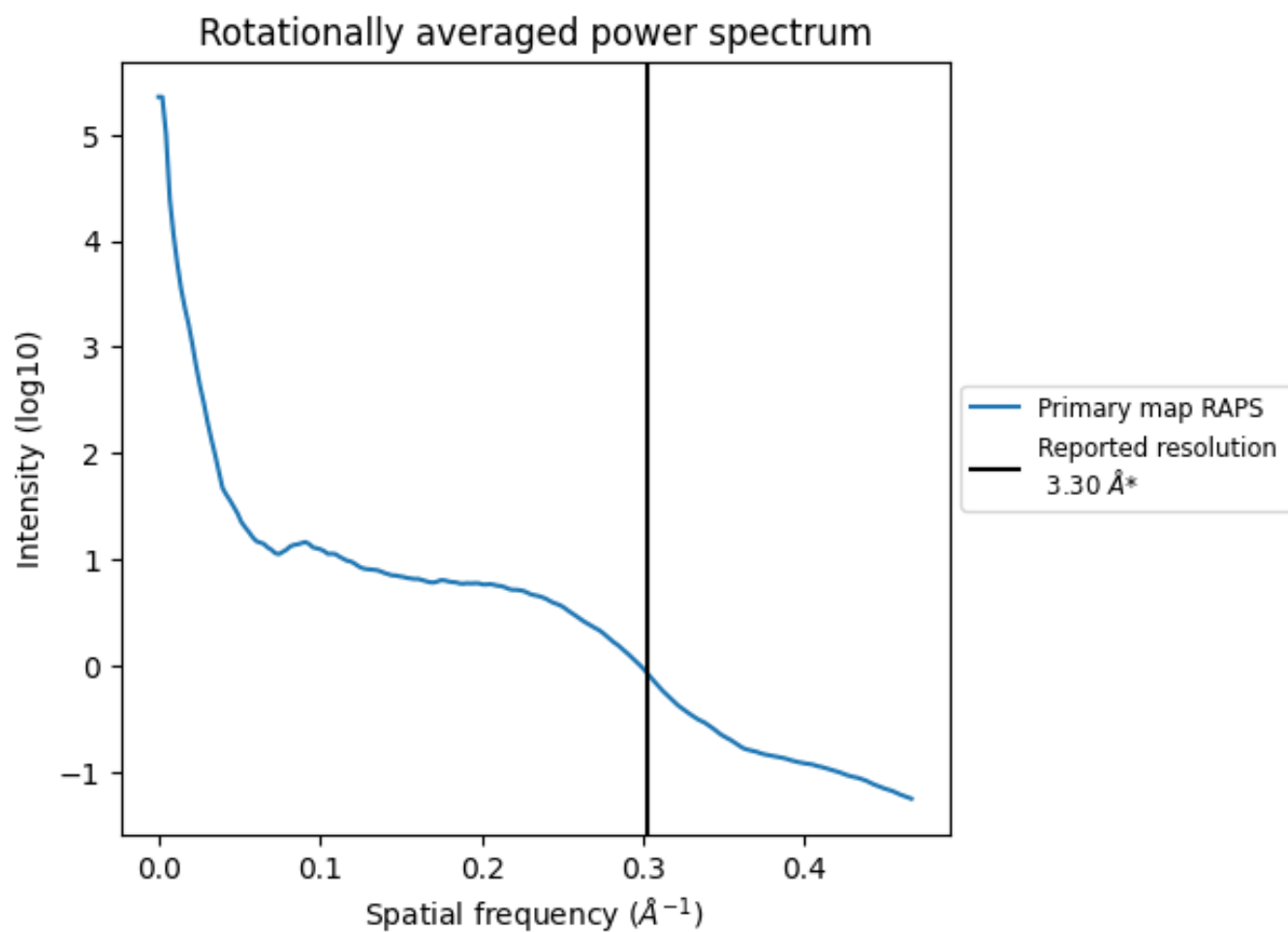
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 256 nm³; this corresponds to an approximate mass of 231 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

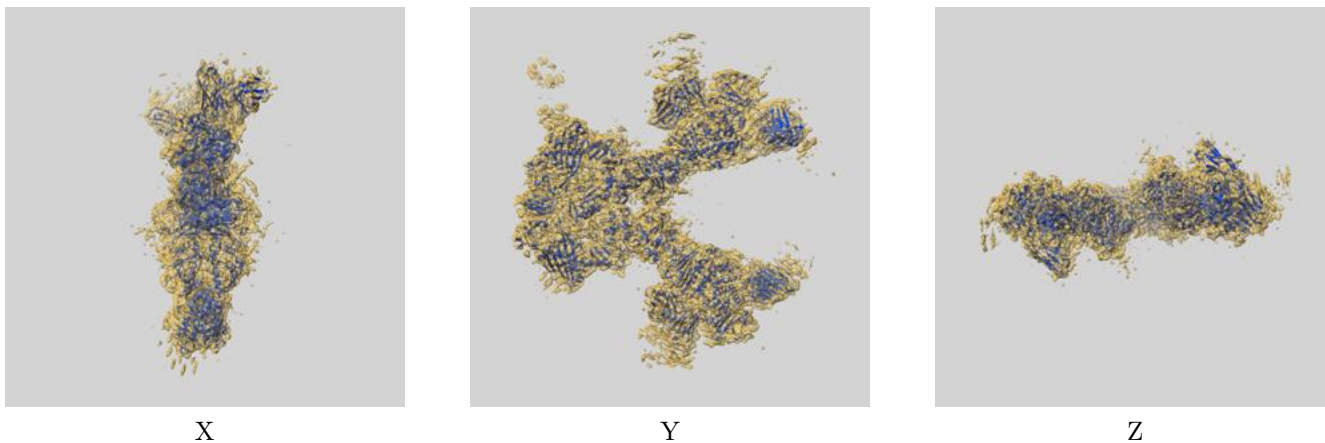
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

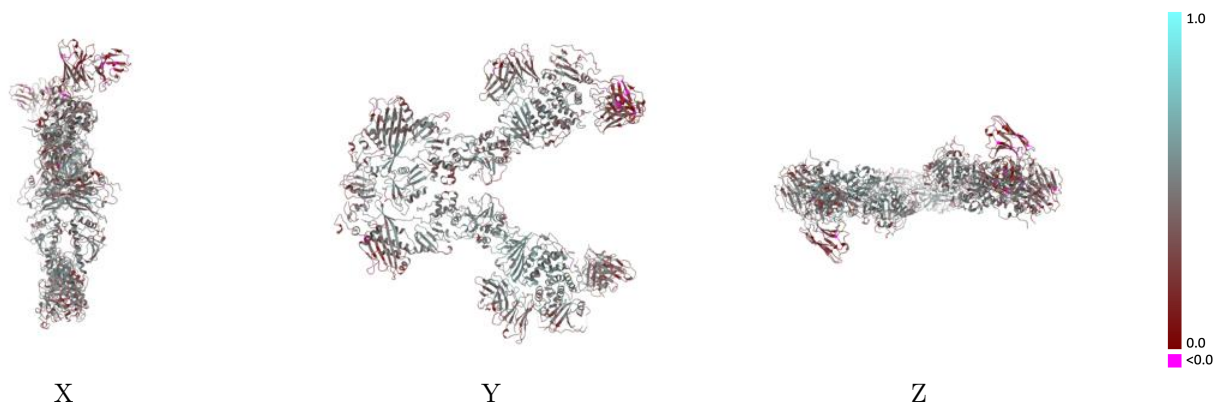
This section contains information regarding the fit between EMDB map EMD-25686 and PDB model 7T4R. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



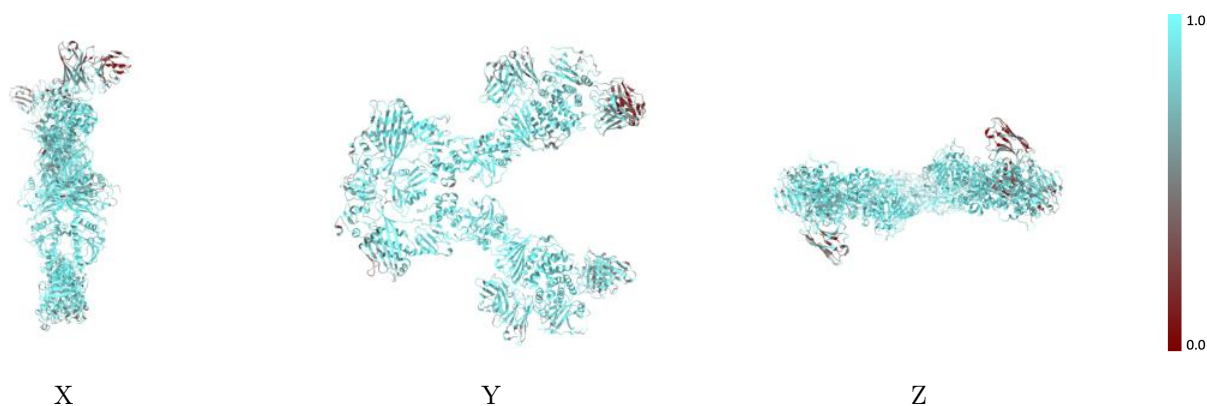
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



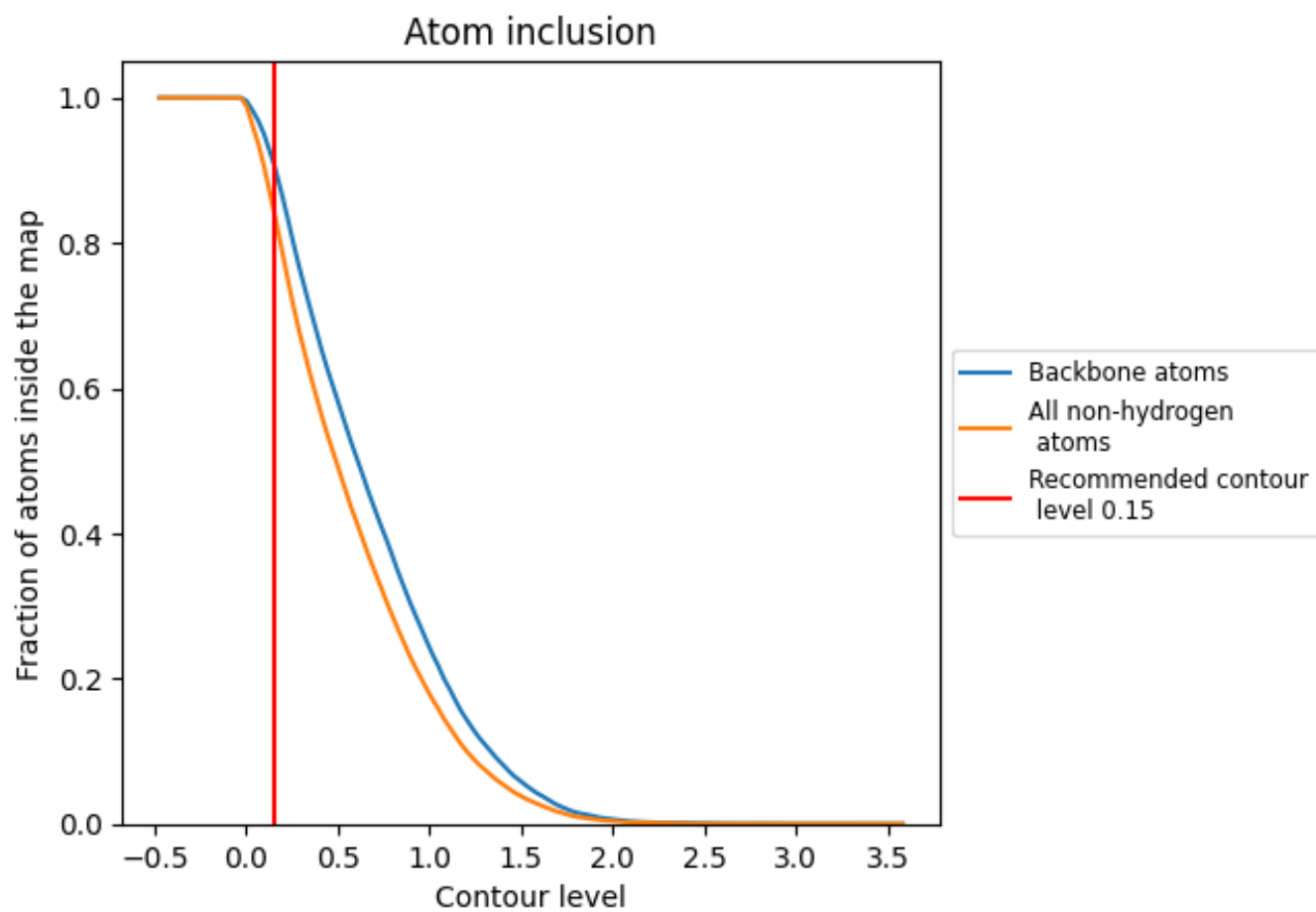
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8450	 0.4290
A	 0.9207	 0.4960
B	 0.8663	 0.4370
C	 0.9096	 0.4390
D	 0.8441	 0.4320
E	 0.8859	 0.4370
F	 0.8353	 0.4160
G	 0.7971	 0.4110
H	 0.7516	 0.3670
I	 0.4970	 0.2440
J	 0.6333	 0.3010
K	 0.9181	 0.4880
L	 0.9439	 0.4920
M	 0.8592	 0.4470
N	 0.8409	 0.4060
O	 0.7550	 0.3650
P	 0.8517	 0.4240
Q	 0.8218	 0.4030
R	 0.6579	 0.3230
S	 0.7917	 0.4010

